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Fractional evolution Dirac-like equations: Some properties and a discrete Von Neumann-type analysis

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ABSTRACT

A system of fractional evolution equations results from employing the tool of the Fractional Calculus and following the method used by Dirac to obtain his well-known equation from Klein–Gordon's one. It represents a possible interpolation between Dirac and diffusion and wave equations in one space dimension.

In this paper some analytical properties typical of the general solution of this system of equations are obtained and necessary stability bounds for a numerical scheme approximating such equations are found, through the classical discrete Von Neumann-type analysis.

The non-local property of the time fractional differential operator leads to discretizations in terms of series. Here, the analytical methods, usually employed in the study of the stability of discrete schemes when dealing with integer order differential equations, have been adapted to the complexity of the real order case.

1. Introduction

In this paper, we will consider a generalization of the linear one-dimensional diffusion and wave equations, that we call "fractional evolution Dirac-like equations". They are obtained by combining the fractional derivatives and the internal degrees of freedom associated to a system, as we will explain below.

The Fractional Calculus (see [4,14,15], for example) deals with the theory of real (or imaginary) order integral and differential operators and it represents a natural instrument to model non-local phenomena, either in space or time, involving different scales.

The general fractional derivative in the variable x can be denoted by D_x^α, where $\alpha > 0$, $\alpha \in \mathbb{R}$, and it must coincide with the classical derivatives for integer orders α. Many different definitions have been proposed in the literature, all preserving this property. Here, we will refer to two of them, especially employed in the mathematical and physical fields.

The first is the Riemann–Liouville fractional derivative of order $\alpha > 0, \alpha \in \mathbb{R}$ (see [15], for example) of a function f given in $[a, b]$, where $[a, b] \subset \mathrm{R}$, $n \in \mathbb{N}$, $n = -[-\alpha]$ and $x > a$:

$$({}_a^{RL}D_x^\alpha f)(x) = \frac{\mathrm{d}^n}{\mathrm{d}x^n}\frac{1}{\Gamma(n-\alpha)}\int_a^x \frac{f(\tau)}{(x-\tau)^{\alpha-n+1}}\mathrm{d}\tau. \tag{1}$$

The second one is the Caputo fractional derivative, which can be considered as a regularised version of the previous definition, since it takes the form

$$({}_a^{C}D_x^\alpha f)(x) = \frac{1}{\Gamma(n-\alpha)}\int_a^x \frac{f^n(\tau)}{(x-\tau)^{\alpha-n+1}}\mathrm{d}\tau. \tag{2}$$

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The following relation between the above definitions holds:

$$({}_a^C D_x^\alpha f)(x) = ({}^{RL}D_{a+}^\alpha f)(x) - \sum_{j=0}^{n-1} \frac{f^{(j)}(a+)}{\Gamma(1+j-\alpha)}(x-a)^{j-\alpha}, \tag{3}$$

and a sufficient condition under which both derivatives exist is $f \in AC^{n-1}(a,b)$ and $f^n(x) \in L^1(a,b)$. Property (3) allows to establish the equivalence between null fractional and classical initial conditions. In fact, if (3) is valid, then:

$$({}^{RL}D_{a+}^\alpha f)(a+) = 0 \iff f^{(j)}(a+) = 0, \quad j = 0, 1, 2, \ldots, n-1. \tag{4}$$

Among the most important differences between the Riemann–Liouville and the Caputo type derivative is the fact that the first one is not zero when calculated on a constant function, whereas the second one is. This analogy with the classical derivative represents one of the main motivations which led Caputo in 1967 [1] to introduce in his studies about applied problems the operator (2) as an alternative to the Riemann–Liouville operator.

Another important distinction between the Riemann-Lioville and the Caputo operator is their behavior under the Laplace transform. In fact, assuming certain restrictions on the function $f(t) : \mathbb{R}_+ \to \mathbb{C}$ such that the following expressions exist, it results:

$$\int_0^\infty \mathrm{e}^{-st} \left(({}^{RL}D_0^\alpha f)(t)\right) \mathrm{d}t = s^\alpha (\mathcal{L}_t f)(s) - \sum_{k=0}^{n-1} s^k ({}^{RL}D_0^{\alpha-k-1} f)(0), \tag{5}$$

$$\int_0^\infty \mathrm{e}^{-st} \left(({}^{C}D_0^\alpha f)(t)\right) \mathrm{d}t = s^\alpha (\mathcal{L}_t f)(s) - \sum_{k=0}^{n-1} s^{\alpha-k-1} f^{(k)}(0), \tag{6}$$

where $s \in \mathbb{C}$ and $\mathcal{L}_t f$ is the Laplace transform of the function f.

Property (6) allows us to employ initial conditions of the classical type with the usual interpretation when solving applied problems through the Laplace transform, which is one of the most recurring method in the physical field due to its easy of use.

Let us now define the fractional evolution Dirac-like equations. It is important to highlight that in the construction of such a generalization of the linear one dimensional diffusion and wave equations, the definition of the fractional operator does not need to be specified from the very beginning. In fact, we will just have to know the fractional operator we are referring to when we want to calculate the solutions of the corresponding specific fractional evolution equations.

As it is known, the free Dirac equation is, in some sense, the square root of the Klein–Gordon equation (see, e.g., [17]). Similarly, we can consider a kind of square root of the following fractional diffusion equation in one space dimension:

$$(D_t^{2\alpha} u)(t,x) - \lambda^2 \partial_{xx} u(t,x) = 0, \tag{7}$$

which has been widely studied in the literature (see [7–10,16], for example).

To do that, let us consider the general system of fractional evolution Dirac-like equations

$$\left(\mathbf{A} D_t^\alpha + \lambda \mathbf{B} \partial_x\right) \mathbf{v}(t,x) = \mathbf{0}, \qquad \mathbf{v}(t,x) = \begin{pmatrix} u_1(t,x) \\ u_2(t,x) \end{pmatrix}, \tag{8}$$

with $0 < \alpha \leq 1$, $\alpha \in \mathbb{R}$, $\lambda \in \mathbb{R}$, $\lambda \neq 0$ and where $\mathbf{A}$ and $\mathbf{B}$ are 2×2 matrixes satisfying the Pauli's algebra:

$$\mathbf{A}^2 = \mathbf{I}, \qquad \mathbf{B}^2 = -\mathbf{I}, \qquad \mathbf{AB} + \mathbf{BA} = \mathbf{0} \tag{9}$$

and $\mathbf{I}$ is the identity matrix.

Each component of the solution $\mathbf{v}(t,x)$ also solves (7) provided the index property

$$({D_t}^\alpha {D_t}^\alpha)\mathbf{v}(t,x) = {D_t}^{2\alpha}\mathbf{v}(t,x) \tag{10}$$

holds.

Actually, under the assumption (10), it turns out that:

$$\begin{aligned} &\left(\mathbf{A} D_t^\alpha + \lambda \mathbf{B} \partial_x\right) \mathbf{v}(t,x) = \mathbf{0} \quad \Longrightarrow \\ &\left(\mathbf{A} D_t^\alpha + \lambda \mathbf{B} \partial_x\right)^2 \mathbf{v}(t,x) = \begin{cases} (D_t^{2\alpha} u_1)(t,x) - \lambda^2 \partial_{xx} u_1(t,x) = 0 \\ (D_t^{2\alpha} u_2)(t,x) - \lambda^2 \partial_{xx} u_2(t,x) = 0. \end{cases} \end{aligned} \tag{11}$$

Observe that, for the fractional Riemann–Liouville and Caputo derivatives the semigroup property (10) occurs when $\mathbf{v}(0,x) = \mathbf{0}$.

In fact, the following proposition holds (see, e.g., [14,15]):

Proposition 1. *Let $\alpha > 0$, $\beta > 0$, $n = -[-\alpha]$, $m = -[-\beta]$ and $x > a$. Given $f \in L^1(a, b)$ such that $(I_{a+}^{m-\beta} f) \in AC^{m-1}[a, b]$ and $(I_{a+}^{n-(\alpha+\beta)} f) \in AC^{n-1}[a, b]$ if $(\alpha + \beta) < n$, or $(I_{a+}^{[\alpha+\beta]} f) \in AC^{[\alpha+\beta]}[a, b]$ if $(\alpha + \beta) > n$, then*

$$({}^{RL}D_{a+}^{\alpha}\, {}^{RL}D_{a+}^{\beta} f)(x) = ({}^{RL}D_{a+}^{\alpha+\beta} f)(x) - \sum_{j=1}^{m} ({}^{RL}D_{a+}^{\beta-j} f)(a+) \frac{(x-a)^{-j-\alpha}}{\Gamma(1-j-\alpha)}, \tag{12}$$

for almost every $x \in [a, b]$.

Here, $\{\alpha + \beta\}$ is the decimal part of $(\alpha + \beta)$. Moreover, given $f \in L^1(a, b)$:

$$\left(I_{a+}^{\alpha} f\right)(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x - z)^{\alpha-1} f(z) \mathrm{d}z, \quad (x > a) \tag{13}$$

is the Riemann–Liouville integral operator of real order $\alpha > 0$.

Therefore, neither the Riemann–Liouville nor the Caupto derivatives (due to (3)) have, in general, the semigroup property but when

$$\left[{}^{RL}D_{a+}^{\beta-j} f\right](a+) = 0, \quad j = 1, 2, \ldots, m, \tag{14}$$

or equivalently, if (4) holds, when

$$f^{(j)}(a+) = 0, \quad j = 0, 1, 2, \ldots, m-1. \tag{15}$$

Thus, when $1/2 < \alpha < 1$ and (10) is fulfilled, system (8) represents a fractional interpolation between diffusion ($\alpha = 1/2$) and wave ($\alpha = 1$) equations.

Solutions of this system could model the diffusion of particles whose behavior depends on the space and time coordinates, as usual, but also on their internal structures.

The first formulation involving the mathematical operation of semi-differentiation in replacement of the Fick's law appeared in [11]. Later, system (8) was studied in ([20], [22,5,12]).

To attribute physical meaning to system (8), we will focus our study on pure real matrixes of Pauli's type leading to non-equivalent systems (8). Just two pairs of matrixes fulfill these requirements:

$$\mathbf{A_1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{B_1} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{16}$$

$$\mathbf{A_2} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathbf{B_2} = \mathbf{B_1} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{17}$$

System

$$\left(\mathbf{A_1} D_t^{\alpha} + \lambda \mathbf{B_1} \partial_x\right) \mathbf{v}(t, x) = \mathbf{0}, \tag{18}$$

is made up of the following equations of uncoupled variables u_1 and u_2:

$$(D_t^{\alpha} u_1)(t, x) - \lambda \partial_x u_1(t, x) = 0, \tag{19}$$

$$(D_t^{\alpha} u_2)(t, x) + \lambda \partial_x u_2(t, x) = 0. \tag{20}$$

System

$$\left(\mathbf{A_2} D_t^{\alpha} + \lambda \mathbf{B_2} \partial_x\right) \mathbf{v}^*(t, x) = \mathbf{0} \tag{21}$$

involves equations of coupled variables u_1^* and u_2^*:

$$(D_t^{\alpha} u_1^*)(t, x) + \lambda \partial_x u_2^*(t, x) = 0, \tag{22}$$

$$(D_t^{\alpha} u_2^*)(t, x) + \lambda \partial_x u_1^*(t, x) = 0. \tag{23}$$

Section 2 of this paper shows how solutions u_1^* and u_2^* of (22) and (23) can be obtained as a linear combination of u_1 and u_2, solutions of (19) and (20), independently from the definition of the fractional derivative one chooses. This allows us to reduce the study concerning the general real system (8) to the case when it is given by (18).

In Section 3 we will refer to a specific fractional differential operator when searching for stability bounds of a numerical scheme approximating the fractional evolution-diffusion equation

$$(D_t^{\alpha} u)(t, x) + \lambda \partial_x u(t, x) = 0. \tag{24}$$

Concretely, we will first find these bounds for the equation

$$({}_0^C D_t^\alpha u)(t,x) + \lambda \partial_x u(t,x) = 0 \tag{25}$$

in the domain $x > a$, $t > 0$ and together with initial and boundary conditions

$$u(0+,x) = u_0(x), \quad x > a, \tag{26}$$

$$u(t,a+) = r(t), \quad t > 0, \tag{27}$$

where $a \in \mathbb{R}$, $u_0(x)$ and $r(t)$ are known functions, and $0 < \alpha < 1$. Later, it will be remarked that the same stability bounds hold when the Riemann–Liouville derivative is employed in the evolution equation (25) instead of the Caputo's one.

We will make use of a convolution quadrature formula proposed in [2] to approximate both the Caputo and the Riemann–Liouville time fractional derivatives and an usual finite difference formula for the space partial derivative. Then, the stability bounds of this scheme will be obtained by means of a discrete Von Neumann-type analysis.

These bounds for the evolution equation with the Caputo derivative are confirmed by a dispersion–dissipation study in Section 4, and they are finally checked in Section 5 for some representative examples, when we know the underlying exact analytical results.

As far as we know, these techniques have not previously appeared in the literature to analyze a discretization of a fractional differential equation. They represent a fundamental tool in the study of the stability of a numerical scheme; so it could be very useful to know how to adapt them to this non-local case.

Finally, as a general remark, it should be highlighted that the same theoretical construction we made above, making use of the fractional derivatives and the Pauli's matrixes to obtain a kind of square root of a differential equation, could be repeated for a differential equation of any integer or real order in time and/or space. Besides, also different orders of the roots, as cubic for instance [20,22], could be considered.

This approach would allow us to study "from an internal point of view" lots of the equations appearing in applied fields, thus providing an additional information on the associated phenomena.

2. Uncoupled and coupled solutions of the system of fractional evolution-diffusion Dirac-like equations

In this section we will prove the relation existing between the coupled solutions of Eqs. (22) and (23), denoted by u_1^* and u_2^*, and the uncoupled solutions u_1 and u_2 of Eqs. (19) and (20).

To do that, let us find two real matrixes

$$\mathbf{M} = \begin{pmatrix} m_1 & m_2 \\ m_3 & m_4 \end{pmatrix}, \qquad \mathbf{N} = \begin{pmatrix} n_1 & n_2 \\ n_3 & n_4 \end{pmatrix}$$

such that

$$\mathbf{A_1} = \mathbf{M}\mathbf{A_2}\mathbf{N}, \qquad \mathbf{B_1} = \mathbf{M}\mathbf{B_2}\mathbf{N}. \tag{28}$$

After few calculations, it is established that conditions (28) imply $m_1 = -m_2, m_3 = m_4, n_1 = -n_3 = \frac{1}{2m_3}, n_2 = n_4 = \frac{1}{2m_1}$, where m_1 and m_3 have to be real numbers different from zero. Then:

$$\mathbf{M} = \begin{pmatrix} m_1 & -m_1 \\ m_3 & m_3 \end{pmatrix}, \qquad \mathbf{N} = \frac{1}{2}\begin{pmatrix} 1/m_3 & 1/m_1 \\ -1/m_3 & 1/m_1 \end{pmatrix}.$$

Now, we can enunciate the following result:

Theorem 2. *The vector* $\mathbf{v}$ *is solution of* (18) *if and only if* $\mathbf{v}^* = \mathbf{N}\mathbf{v}$ *is solution of* (21).

Proof. It is sufficient to insert relation (28) into (18) to obtain the conclusion as an immediate consequence of the following implication

$$\left(\mathbf{A_1} D_t^\alpha + \lambda \mathbf{B_1} \partial_x\right) \mathbf{v}(t,x) = \mathbf{0} \Leftrightarrow \left(\mathbf{A_2}\mathbf{N} D_t^\alpha + \lambda \mathbf{B_2}\mathbf{N}\partial_x\right) \mathbf{v}(t,x) = \mathbf{0}. \quad \blacksquare$$

Note that, according to Theorem 2, when dealing with the analytical aspects of system (8) we can restrict ourselves to study (18). Actually, if u_1 is the solution of (19) and u_2 the solution of (20), then:

$$u_1^* = (c_1 u_1 + c_2 u_2), \tag{29}$$

$$u_2^* = (c_2 u_2 - c_1 u_1), \tag{30}$$

solve, respectively, Eqs. (22) and (23) for every nonzero real constants c_1 and c_2.

Before concluding this section, it is worth noting that the result stated in Theorem 2 is independent from the definition of the fractional derivative operator appearing in Eqs. (18) and (21). Also, it should be emphasized that it is still valid whenever one wanted to extend our technique to consider the same kind of square root of an equation *of any real order* by means of the Pauli's matrixes, as we did above.

3. Construction of the numerical scheme

The most important feature of a fractional derivative that has to be taken into account when constructing a numerical scheme is its non-local property. This characteristic leads to discretizations consisting of a lower triangular matrix instead of a multi-diagonal matrix, as in the case of integer order classical derivatives.

In fact, suppose $t \in [0, T]$, $x \in [a, b]$, and introduce the temporal nodes $t_n = n\Delta t$, where $n = 0, \ldots, N$, $t_0 = 0$, $t_N = T$, and the spatial nodes $x_l = a + l\Delta x$ where $l = 0, \ldots, M$, $x_0 = a$ and $x_M = b$. Then the Riemann–Liouville fractional derivative can be approximated as follows:

$$\begin{pmatrix} ({}_0^{RL}D_t^{\alpha}\, u)(t_0, x) \\ ({}_0^{RL}D_t^{\alpha}\, u)(t_1, x) \\ \vdots \\ ({}_0^{RL}D_t^{\alpha}\, u)(t_N, x) \end{pmatrix} \approx \frac{1}{\Delta t^{\alpha}} \begin{pmatrix} \omega_{0,0} & 0 & \cdots & \cdots 0 \\ \omega_{1,0} & \omega_{1,1} & 0 & \cdots 0 \\ \vdots & \vdots & \ddots & \ddots 0 \\ \omega_{N,0} & \cdots & \cdots & \omega_{N,N} \end{pmatrix} \begin{pmatrix} u(t_0, x) \\ u(t_1, x) \\ \vdots \\ u(t_N, x) \end{pmatrix}.$$

Here we write Δt^{α} instead of $(\Delta t)^{\alpha}$ for simplicity.

In an equivalent form, the value of the Riemann–Liouville derivative for each time-space point (t_n, x_l) can be approximated by

$$({}_0^{RL}D_{t_n}^{\alpha}\, u)(t_n, x_l) \approx \frac{1}{\Delta t^{\alpha}} \sum_{j=0}^{n} \omega_{n,j} u_l^j, \tag{31}$$

where u_l^n is the numerical approximation of $u(t_n, x_l)$, $u_0^n = u(t_n, a) = r(t_n)$ and $u_l^0 = u(0, x_l) = u_0(x_l)$.

Due to (3), the corresponding approximation for the Caputo derivative is

$$({}_0^{C}D_{t_n}^{\alpha}\, u)(t_n, x_l) \approx \frac{1}{\Delta t^{\alpha}} \sum_{j=0}^{n} \omega_{n,j} u_l^j - \frac{t_n^{-\alpha} u_0(x_l)}{\Gamma(1-\alpha)}. \tag{32}$$

In this paper we employ the convolution quadrature formula (31) where we deduce $\omega_{n,j}$ from the the weights proposed in [2]:

$$\Gamma(2-\alpha)\omega_{n,j} = \begin{cases} 1 & j = n \\ (n-j-1)^{1-\alpha} - 2(n-j)^{1-\alpha} + (n-j+1)^{1-\alpha} & 1 \le j \le n-1 \\ (n-1)^{1-\alpha} - (\alpha-1)n^{-\alpha} - n^{1-\alpha} & j = 0. \end{cases} \tag{33}$$

It has been shown in [2] that the convergence order associated to this formula is $O(\Delta t)^{2-\alpha}$.

As well, the weights obtained by Lubich in [6] by means of the so called *discretized operational calculus* could have been used instead of (33). However, such weights lead to an approximation for the Riemann–Liouville derivative with a convergence order $O(\Delta t)^{\alpha}$. So, as in our case the index of the fractional derivative in time varies between 0 and 1, Diethelm's weights turn out to be advantageous.

In combination with the discrete formula involving Diethelm's weights for the time fractional derivative, we employ a classical forward Euler formula to approximate the first order space derivative:

$$\partial_x u(t_n, x_l) \approx \frac{u_{l+1}^n - u_l^n}{\Delta x}. \tag{34}$$

Therefore, the finite difference equation corresponding to (25) is:

$$u_{l+1}^n = \left(1 - \omega_{n,n} \frac{\Delta x}{\lambda \Delta t^{\alpha}}\right) u_l^n + \frac{\Delta x}{\lambda} \left[\frac{u_0(x_l) t_n^{-\alpha}}{\Gamma(1-\alpha)} - \sum_{j=0}^{n-1} \frac{\omega_{n,j}}{\Delta t^{\alpha}} u_l^j\right], \tag{35}$$

for all $l = 0, \ldots, M-1$ and $n = 1, \ldots, N$. It can be proved that the error associated to this formula is $O(\Delta t)^{2-\alpha} + O(\Delta x)$.

Now, let us present the main result on the stability obtained from the discrete Von Neumann-type analysis of the scheme (35) together with initial condition (26).

Theorem 3. *Given the numerical scheme (35) approximating the fractional evolution equation (25) together with the initial condition (26), a necessary condition for the scheme to be stable for all $\alpha \in (0, 1)$ is:*

$$\frac{\Delta x}{\lambda \Delta t^{\alpha} \Gamma(2-\alpha)} \le 1. \tag{36}$$

Proof. Let us introduce in Eq. (35) the discrete Fourier mode

$$u_l^n = \tau^n e^{ilQ\Delta x}, \tag{37}$$

where it is assumed $Q = m\pi$, being m an integer such that $0 \le m \le M$, and the super index of τ stands for its n-th power. Then, after dividing by $e^{ilQ\Delta x}$ and considering that $t_n = n\Delta t$, it results

$$\tau^n \left(e^{iQ\Delta x} - 1 + \frac{\Delta x}{\lambda \Delta t^\alpha \Gamma(2-\alpha)} \right) = -\sum_{j=0}^{n-1} \bar{\omega}_{n,j} \tau^j \tag{38}$$

where

$$\bar{\omega}_{n,j} = \begin{cases} -\dfrac{\Delta x \left((n-j)^{1-\alpha} - (n-j-1)^{1-\alpha} - ((n-j+1)^{1-\alpha} - (n-j)^{1-\alpha}) \right)}{\lambda \Delta t^\alpha \Gamma(2-\alpha)} & j = 1, \ldots, n-1 \\ -\dfrac{\Delta x \left(n^{1-\alpha} - (n-1)^{1-\alpha} \right)}{\lambda \Delta t^\alpha \Gamma(2-\alpha)} & j = 0. \end{cases} \tag{39}$$

Also, let us fix the simple notations

$$L(Q) = \left(e^{iQ\Delta x} - 1 + \frac{\Delta x}{\lambda \Delta t^\alpha \Gamma(2-\alpha)} \right), \tag{40}$$

and

$$A_\alpha = \frac{\Delta x}{\lambda \Delta t^\alpha \Gamma(2-\alpha)}. \tag{41}$$

Now, we can show the following property of the coefficients (39), which is relevant in our proof:

$$\sum_{j=0}^{n-1} -\bar{\omega}_{n,j} = \sum_{j=0}^{n-1} \left| \bar{\omega}_{n,j} \right| = A_\alpha, \quad \forall n = 1, 2, \ldots. \tag{42}$$

In fact, it results:

$$-\bar{\omega}_{1,0} = \left| \bar{\omega}_{1,0} \right| = A_\alpha, \quad \text{if } n = 1,$$

and we have

$$\begin{aligned} &-\bar{\omega}_{n,0} - \bar{\omega}_{n,1} = A_\alpha(-(n-2)^{1-\alpha} + (n-1)^{1-\alpha}) \quad \text{if } n \ge 2, n \in \mathbb{N}, \\ &-\bar{\omega}_{n,0} - \bar{\omega}_{n,1} - \bar{\omega}_{n,2} = A_\alpha(-(n-3)^{1-\alpha} + (n-2)^{1-\alpha}) \quad \text{if } n \ge 3, n \in \mathbb{N}, \\ &-\bar{\omega}_{n,0} - \bar{\omega}_{n,1} - \bar{\omega}_{n,2} - \bar{\omega}_{n,3} = A_\alpha(-(n-4)^{1-\alpha} + (n-3)^{1-\alpha}) \quad \text{if } n \ge 4, n \in \mathbb{N}, \\ &\vdots \end{aligned}$$

so that, in general, it is:

$$\sum_{j=0}^{n-1} -\bar{\omega}_{n,j} = A_\alpha(-(n-n)^{1-\alpha} + (n-(n-1))^{1-\alpha}) = A_\alpha \quad \forall n \ge 2.$$

Now, when $n = 1$:

$$|\tau(Q)| = \frac{-\bar{\omega}_{1,0}}{|L(Q)|} = \frac{A_\alpha}{|L(Q)|} \tag{43}$$

and then

$$\frac{A_\alpha}{1 + |1 - A_\alpha|} \le |\tau(Q)| \le \frac{A_\alpha}{|1 - |1 - A_\alpha||} \quad \forall Q, \tag{44}$$

being:

$$|1 - |1 - A_\alpha|| \le |L(Q)| \le 1 + |1 - A_\alpha|, \quad \forall Q. \tag{45}$$

Therefore:

$$|\tau(Q)| \leq 1 \quad \forall Q, \text{ if } A_\alpha < 1, \tag{46}$$

$$|\tau(Q)| \geq 1 \quad \forall Q, \text{ if } A_\alpha > 1, \tag{47}$$

$$|\tau(Q)| = 1 \quad \forall Q, \text{ if } A_\alpha = 1, \tag{48}$$

since $\frac{A_\alpha}{|1-|1-A_\alpha||} = 1$ if $A_\alpha \leq 1$, and $\frac{A_\alpha}{1+|1-A_\alpha|} = 1$ if $A_\alpha \geq 1$.

When $n \neq 1$, e.g. $n = 2$, we have from (38) that:

$$\tau^2 = \frac{1}{L(Q)}(-\bar{\omega}_{2,0} - \bar{\omega}_{2,1}\tau) \tag{49}$$

and so it is preserved that

$$|\tau(Q)|^2 \leq \frac{1}{|L(Q)|}(|\bar{\omega}_{2,0}| + |\bar{\omega}_{2,1}|) = \frac{A_\alpha}{|L(Q)|} \leq 1 \quad \forall Q, \text{ if } A_\alpha \leq 1,$$

by (42).

Repeating the same, for the general case $n \neq 1$, $n \in \mathbb{N}$, we still obtain:

$$|\tau(Q)|^n \leq \frac{1}{|L(Q)|}\sum_{j=0}^{n-1}|\bar{\omega}_{n,j}|\,|\tau(Q)|^j \leq \frac{1}{|L(Q)|}\sum_{j=0}^{n-1}|\bar{\omega}_{n,j}| = \frac{A_\alpha}{|L(Q)|} \leq 1 \quad \forall Q, \text{ if } A_\alpha \leq 1. \tag{50}$$

Therefore, if we impose $|\tau(Q)| \leq 1$ for all Q (and all $n \in \mathbb{N}$) in order to obtain the necessary condition for the stability of the numerical scheme (35) (see [18], for example), it is evident that here this restriction, called the discrete Von Neumann's criterion, is fulfilled whenever $A_\alpha \leq 1$. ■

Remark 4. The classical discrete Von Neumann-type analysis that we realized only allows us to find a pure necessary condition for the stability which, in general, is not sufficient.

To obtain both a necessary and sufficient condition of stability, a discrete generalized Von Neumann-type analysis should be derived, not based on the usual Fourier mode (37), but on some appropriate functions deduced by applying discrete method of separation of variables to the problem under study (see [18, Chapt. 3]). Also, a different method taking boundary conditions into account and leading to stronger conditions of stability is the so-called "GKSO", detailed in [19].

We want to underline that (36) returns the classical conditions for stability in the limiting cases $\alpha = 0$ and $\alpha = 1$.

In fact, due to (3), the fractional evolution-diffusion equation (25) can be rewritten as follows

$$({}_0^{RL}D_t^\alpha u)(t,x) - \frac{u_0(x)t^{-\alpha}}{\Gamma(1-\alpha)} + \lambda\partial_x u(t,x) = 0, \tag{51}$$

and, holding $({}_0^{RL}D_t^1 u)(t,x) = \partial_t u(t,x)$ and $({}_0^{RL}D_t^0 u)(t,x) = u(t,x)$, it is reduced to

$$\partial_t u(t,x) + \lambda\partial_x u(t,x) = 0, \tag{52}$$

when $\alpha = 1$, whereas it is given by equation

$$u(t,x) - u_0(x) + \lambda\partial_x u(t,x) = 0, \tag{53}$$

when $\alpha = 0$.

Now, when $\alpha = 1$, $\omega_{n,j} = 0$ for all $j = 0, 1, \ldots, n-2$ and $\omega_{n,n} = 1$, $\omega_{n,n-1} = -1$. Moreover, when $\alpha = 0$, $\omega_{n,j} = 0$ for all $j = 0, 1, \ldots, n-1$ and $\omega_{n,n} = 1$. So, the finite difference Eq. (35), when $\alpha = 1$, reads

$$u_{l+1}^n = \left(1 - \frac{\Delta x}{\lambda\Delta t}\right)u_l^n + \frac{\Delta x}{\lambda\Delta t}u_l^{n-1}, \tag{54}$$

being $\frac{u_0(x_l)t_n^{-\alpha}}{\Gamma(1-\alpha)}|_{\alpha=1} = 0$, whereas, when $\alpha = 0$, it is the following:

$$u_{l+1}^n = \left(1 - \frac{\Delta x}{\lambda}\right)u_l^n + \frac{\Delta x}{\lambda}u_0(x_l). \tag{55}$$

Schemes (54) and (55) are exactly the ones we would obtain by applying forward Euler formulas to discretize the first order derivatives in space and time appearing in (52), and just the first order space derivative included in (53), respectively.

Von Neumann-type analysis of stability of scheme (54) leads to:

$$\tau^n\left(e^{iQ\Delta x} - 1 + \frac{\Delta x}{\lambda\Delta t}\right) = \frac{\Delta x}{\lambda\Delta t}\tau^{n-1}, \tag{56}$$

which is equivalent to

$$\tau(Q) = \left[\frac{A_1}{\left(e^{iQ\,\Delta x} - 1 + A_1\right)} \right], \tag{57}$$

where $A_1 = \Delta x/(\lambda \Delta t) = A_\alpha|_{\alpha=1}$.

From this, the inequality

$$|\tau(Q)| \leq \frac{|A_1|}{|1 - |1 - A_1||}, \qquad \forall Q, \tag{58}$$

is deduced and therefore, according to the Von Neumann's criterion, a necessary condition for the stability of scheme (54) is $A_1 = \Delta x/(\lambda \Delta t) \leq 1$.

On the other hand, when $\alpha = 0$ the discrete Von Neumann's analysis of stability for the scheme (54) leads to the following equation:

$$\tau^n \left(e^{iQ\,\Delta x} - 1 + \frac{\Delta x}{\lambda} \right) = \frac{\Delta x}{\lambda}, \tag{59}$$

or, equivalently, to

$$\tau(Q) = \left[\frac{A_0}{\left(e^{iQ\,\Delta x} - 1 + A_0\right)} \right]^{1/n}, \tag{60}$$

where $A_0 = \Delta x/\lambda = A_\alpha|_{\alpha=0}$.

So, the following inequality can be written:

$$|\tau(Q)| \leq \left[\frac{|A_0|}{|1 - |1 - A_0||} \right]^{1/n}, \quad \forall Q, \tag{61}$$

and, again, the necessary condition of stability for the scheme (55) is obtained by imposing $|\tau(Q)| \leq 1\ \forall Q$, that leads to $A_0 = \Delta x/\lambda \leq 1$.

We finally conclude this section with the following remark. The same bounds (36) hold for the evolution equation:

$$({}_0^{RL}D_t^\alpha\, u)(t, x) + \lambda \partial_x u(t, x) = 0 \tag{62}$$

in the domain $x > a$, $t > 0$ and together with the initial condition

$$\lim_{t \to 0} (I_0^{1-\alpha} u)(t, x) = u_0(x), \quad x > a. \tag{63}$$

In fact, according to (31), the finite difference equation corresponding to (62) is:

$$u_{l+1}^n = \left(1 - \omega_{n,n} \frac{\Delta x}{\lambda \Delta t^\alpha}\right) u_l^n + \frac{\Delta x}{\lambda} \left[-\sum_{j=0}^{n-1} \frac{\omega_{n,j}}{\Delta t^\alpha} u_l^j \right], \tag{64}$$

for all $l = 0, \ldots, M - 1$ and $n = 1, \ldots, N$, and introducing the discrete Fourier mode (37) in it we arrive to the following expression:

$$\tau^n \left(e^{iQ\,\Delta x} - 1 + \frac{\Delta x}{\lambda \Delta t^\alpha\, \Gamma(2 - \alpha)} \right) = -\frac{\Delta x}{\lambda \Delta t^\alpha} \sum_{j=0}^{n-1} \omega_{n,j} \tau^j. \tag{65}$$

Now, being: $-\omega_{1,0} = \alpha/\Gamma(2 - \alpha) < 1/\Gamma(2 - \alpha)$, we have that $|\tau(Q)| < A_\alpha/|L(Q)|\ \forall Q$. As well, $\forall n = 2, 3, \ldots$ it holds that $0 \leq -\omega_{n,0} \leq \alpha/\Gamma(2 - \alpha)$, $-\omega_{n,j} \geq 0$ and

$$\frac{\Delta x}{\lambda \Delta t^\alpha} \sum_{j=0}^{n-1} -\omega_{n,j} = A_\alpha \left[-(1 - \alpha) n^{-\alpha} + 1 \right] < A_\alpha.$$

So repeating the same argumentations as in Theorem 3, we obtain our conclusion.

4. Dispersion–dissipation relation

4.1. Motivation

Usually, while solving analytically a partial differential equation, the dispersion–dissipation relation $\omega = \omega(\beta)$ [21] is pursued so that the following wave in time and space

$$u(t,x) = \hat{u}\mathrm{e}^{\mathrm{i}(\omega t+\beta x)}, \tag{66}$$

where $\hat{u}$ is a constant, is a solution of such an equation (see [18], for instance).

If we consider the parabolic diffusion equation

$$\partial_t u(t,x) - \nu\partial_{xx}u(t,x) = 0 \tag{67}$$

and the hyperbolic evolution equation

$$\partial_t u(t,x) + \lambda\partial_x u(t,x) = 0, \tag{68}$$

then (66) solves (67) if $\omega = i\nu\beta^2$, and (68) whenever $\omega = -\lambda\beta$.

Therefore, the wave solving (67) takes the form

$$u(t,x) = \hat{u}\mathrm{e}^{-\nu\beta^2 t}\mathrm{e}^{\mathrm{i}\beta x}, \tag{69}$$

and it does not move in space whereas it decays in time if $\nu > 0$. This is the typical behavior shown by wave solutions of parabolic type equations.

Likewise, solution (66) of Eq. (68) takes the expression

$$u(t,x) = \hat{u}\mathrm{e}^{\mathrm{i}\beta(x-\lambda t)}, \tag{70}$$

which is a wave propagating along the x axe with a speed $\lambda = -\omega/\beta$ and without any decay in the amplitude. In particular, when ω is a linear function of β, the propagation speed is independent from the frequency.

Decay and propagation of the different Fourier modes are very important to describe the behavior of the solution of a partial differential equation.

In fact, solutions of partial differential equations are said to be *dissipative* when the Fourier modes do not grow in time and one, at least, decays. This is the case, for example, of the solutions (69) of the diffusion equation (67), which all dissipate when $\nu > 0$, except for the constant solution $u(t,x) = \hat{u}$ associated to the wave number $\beta = 0$, that is not well determined by Eq. (67). Solutions are said to be *non-dissipative* when the Fourier modes do not grow nor decay, as it occurs with the waves (70) solving the evolution equation (68).

Finally, solutions of partial differential equations are said to be *dispersive* if the Fourier modes having different wavelengths propagate with different speeds; this is the case, for example, of the solutions of equations just involving partial derivative in x of order equal or bigger than 1.

On the other hand, when a finite difference equation is employed to approximate the continuous solution of a partial differential equation, the behavior of its numerical solution also depends on if the discrete Fourier modes decay or grow. For example, it can be said that the numerical scheme is unstable whenever some modes grow without bounds.

4.2. The fractional case

In the particular case under study in this section, the wave function (66) has to be a solution of the fractional evolution-diffusion Dirac like Eq. (25). Then we obtain a dispersion–dissipation relation much more complex than the which ones appearing in the examples above.

In fact, we have:

$$\begin{aligned} {}_0^C D_t^\alpha\, \hat{u}\mathrm{e}^{\mathrm{i}(\omega t+\beta x)} &= \hat{u}t^{-\alpha}\mathrm{e}^{\mathrm{i}\beta x}E_{1,1-\alpha}(\mathrm{i}\omega t) - \hat{u}\frac{t^{-\alpha}}{\Gamma(1-\alpha)}\mathrm{e}^{\mathrm{i}\beta x} \\ &= \mathrm{i}\omega\hat{u}t^{1-\alpha}\mathrm{e}^{\mathrm{i}\beta x}E_{1,2-\alpha}(\mathrm{i}\omega t), \end{aligned}$$

in view of property (3) and the following:

$$({}_a^{RL}D_x^\alpha\, u)\mathrm{e}^{\lambda x} = \frac{\mathrm{e}^{\lambda a}}{(x-a)^\alpha}E_{1,1-\alpha}(\lambda x - \lambda a) \tag{71}$$

where $\lambda \in \mathbb{R}$ and the definition of the Mittag–Leffler function [3] is

$$E_{\alpha,\beta}(z) = \sum_{j=0}^{\infty}\frac{z^j}{\Gamma(\alpha j+\beta)} = \frac{1}{2\pi\mathrm{i}}\int_{Ha}\frac{\mathrm{e}^\sigma\sigma^{\alpha-\beta}}{\sigma^\alpha - z}\mathrm{d}\sigma. \tag{72}$$

Here $\{\alpha, \beta, z\} \in \mathbb{C}$, $\mathrm{Re}(\alpha) > 0$ and Ha is the Hankel path, a loop which starts from $-\infty$ along the lower side of the negative real axis, encircles the circular disc $|\sigma| \leq |z|^{1/\alpha}$ in the positive sense $|\arg\sigma| \leq \pi$ and ends at $-\infty$ along the upper side of the negative real axis.

So, the dispersion–dissipation relation associated to Eq. (25) is given by the following expression:

$$\omega t^{1-\alpha} E_{1,2-\alpha}(\mathrm{i}\omega t) = -\lambda\beta \mathrm{e}^{\mathrm{i}\omega t}. \tag{73}$$

When $\alpha = 1$, formula (73) coincides with the relation obtained for the evolution equation (68). When $\alpha \neq 1$, it is not possible to obtain explicitly ω as a function of β. It results, in fact, $\omega = \omega(\beta, t)$ due to the non-local character of the fractional differential operator. As a consequence, the dispersion–dissipation relation also involves time.

We consider the behavior of the Fourier modes in solving the numerical scheme (35) associated with Eq. (25).

The first step is to provide the discrete analogous of the Fourier mode (66):

$$u_l^n = \hat{u}\mathrm{e}^{\mathrm{i}\omega n\Delta t}\mathrm{e}^{\mathrm{i}l\beta\Delta x}. \tag{74}$$

Then, as in the continuous case, we search for the relation $\omega = \omega(\beta)$ allowing (74) to be a solution of (35).

According to calculations realized in the proof of Theorem 3, and particularly to (38), we can write

$$\mathrm{e}^{\mathrm{i}\omega\Delta t} = -\frac{\bar{\omega}_{1,0}}{\left(\mathrm{e}^{\mathrm{i}\beta\Delta x} - 1 + A_\alpha\right)} = \frac{A_\alpha}{\left(\mathrm{e}^{\mathrm{i}\beta\Delta x} - 1 + A_\alpha\right)} = \frac{A_\alpha}{L}. \tag{75}$$

Here the weight $\bar{\omega}_{1,0}$ is deduced from (39), the expressions for A_α and L have been given in (41) and (40) (provided Q is substituted by β), respectively.

Now, if we write $\omega = a + ib$, it turns out to be $\mathrm{e}^{\mathrm{i}\omega\Delta t} = \mathrm{e}^{\mathrm{i}a\Delta t}\mathrm{e}^{-b\Delta t}$, where

$$b = -\frac{1}{\Delta t}\ln\frac{|A_\alpha|}{|L|}. \tag{76}$$

Consequently, all the waves given by (74) with $\beta \neq 0$ decay if $b > 0$. This means that the scheme is dissipative if $\frac{|A_\alpha|}{|L|} < 1$, and this is fulfilled if $A_\alpha = \frac{\Delta x}{\lambda\Delta t^\alpha\Gamma(2-\alpha)} < 1$. If $\beta = 0$, the Fourier mode (74) does not grow nor decay and the scheme is not dissipative. Finally, when $\beta \neq 0$ and $b < 0$ ($\frac{|A_\alpha|}{|L|} > 1$), the scheme is unstable because some Fourier modes are unbounded.

Therefore, a necessary condition for the scheme to be stable is exactly the condition (36) provided in Theorem 3.

On the other side, it turns out to be

$$\mathrm{e}^{\mathrm{i}a\Delta t} = \frac{A_\alpha}{L}\frac{|L|}{|A_\alpha|} = \frac{A_\alpha}{|A_\alpha|}\left(\cos(\beta\Delta x) + A_\alpha - 1 - i\sin(\beta\Delta x)\right), \tag{77}$$

and so

$$\tan(a\Delta t) = -\frac{\sin(\beta\Delta x)}{\cos(\beta\Delta x) + A_\alpha - 1}. \tag{78}$$

As a consequence,

$$a = -\frac{1}{\Delta t}\arctan\left(\frac{\sin(\beta\Delta x)}{A_\alpha - 2\sin^2\left(\frac{\beta\Delta x}{2}\right)}\right), \tag{79}$$

and the scheme is dispersive, being this expression not a linear function in β.

Generally speaking, when a numerical scheme shows dissipation and dispersion at the same time, then dissipation uses to hide dispersion and the Fourier modes which try to move at a wrong velocity are muffled. If one wanted to confirm this assumption, then he should study both the behavior of $\mathrm{e}^{-b\Delta t}$, in order to see how the solution dissipates, and of the error in the propagation speed of the Fourier mode involving $\beta\Delta x$, for all $0 \leq \beta\Delta x \leq \pi$. Said error is the difference between the exact propagation speed of the wave (66) solving (25) (represented by the function of β given by $-\omega/\beta$, that we would know explicitly if we could find the explicit expression of ω as a function of β starting from relation (73)) and the speed of propagation of the discrete Fourier mode (74), given by

$$-a/\beta = \frac{1}{\beta\Delta t}\arctan\left(\frac{\sin\beta\Delta x}{A_\alpha - 2\sin^2\frac{\beta\Delta x}{2}}\right),$$

for all $0 \leq \beta\Delta x \leq \pi$.

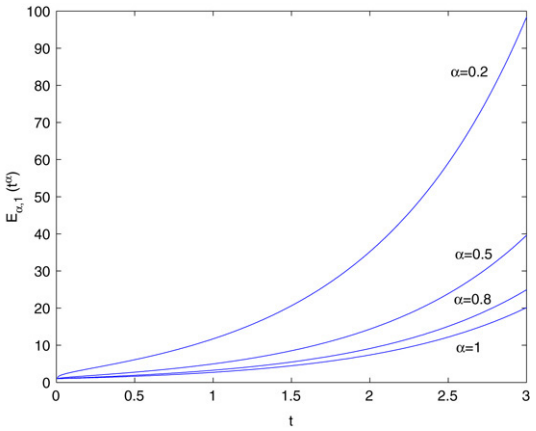

Fig. 1. Function $E_{\alpha,1}\,(t^\alpha)$ for $0 \le t \le 3$ when $\alpha = 0.2, \alpha = 0.5, \alpha = 0.8$ and $\alpha = 1$.

5. Numerical results

To conclude, we show numerical results emerging from simulations of the evolution-diffusion equation (25) together with the specific initial-boundary conditions

$$\begin{aligned} &u(0+,x) = \mathrm{e}^{-\mu x}, \quad x > a, \\ &u(t,a+) = \mathrm{e}^{-\mu a} E_{\alpha,1}(\mu\lambda t^\alpha), \quad t > 0, \end{aligned} \tag{80}$$

where $a \in \mathbb{R}$, $\mu > 0$ and $0 < \alpha < 1$. These simulations employed the scheme (35), in order to check the stability bounds (36).

The analytical solution of this problem was obtained in [13] and it is given by

$$u_\alpha(t,x) = \mathrm{e}^{-\mu x} E_{\alpha,1}(\mu\lambda t^\alpha), \tag{81}$$

for all $x \ge a$ and $t \ge 0$. According to the properties of the Mittag–Leffler function, it takes the specific forms:

$$u_{1/2}(t,x) = \mathrm{e}^{-\mu x}\mathrm{e}^{\mu^2\lambda^2 t}\mathrm{erfc}\left(-\mu\lambda\sqrt{t}\right), \tag{82}$$

$$u_1(t,x) = \mathrm{e}^{-\mu(x-\lambda t)}. \tag{83}$$

In practice, to provide the values of (81), the Mittag–Leffler serie is calculated by solving numerically the ordinary differential equation

$$({}_0^C D_t^\alpha\, u)(t) - \mu\lambda u(t) = 0, \tag{84}$$

with the initial condition $u(0) = 1$, being $E_{\alpha,1}\,(\mu\lambda t^\alpha)$ the exact solution of this problem.

Fig. 1 represents the function $E_{\alpha,1}\,(t^\alpha)$ for $t \in [0, 3]$ and when $\alpha = 0.2, \alpha = 0.5, \alpha = 0.8$ and $\alpha = 1$.

Software Matlab7.0 working in double precision has been used to perform all the numerical simulations.

The following example confirms that condition (36) over time and space steps of the finite difference scheme (35) is necessary in order to have stability. We calculated the maximum of the absolute errors resulting between the values of the exact solution (81), numerically evaluated over the space-time grid points, and the approximate ones produced by the implementation of the difference scheme (35) when $\mu = \lambda = 1, x \in [1, 3.5], \Delta x = 0.025, t \in [0, 2], \Delta t = 0.0125$. Then, we observed that its value is 0.1189 when $\alpha = 0.1$, 0.00241 when $\alpha = 0.5$ and that it is unbounded when $\alpha = 0.9$.

The result concerning $\alpha = 0.9$ is due to the breaking of the condition (36). In fact, relation $(\Delta x/(\Delta t^\alpha \Gamma(2-\alpha))) \le 1$ comes true if $\alpha = 0.1$ and $\alpha = 0.5$, whereas it is not fulfilled when $\alpha = 0.9$, being $\Delta x = 0.025$, $\Delta t^{0.9} = 0.0194$ and $\Gamma(1.1) = 0.9513$. Now, if we simulate the same solutions when $\mu = 1, x \in [1, 3.5], \Delta x = 0.025, t \in [0, 2], \Delta t = 0.0125$, but $\lambda = -1$, we find that the scheme (35) converges only when $\alpha = 0.1$ and it diverges for $\alpha = 0.5$ and $\alpha = 0.9$.

The large number of simulations we performed for different values of α, Δx, Δt and λ indicates that a necessary and sufficient condition ensuring the stability of the difference scheme (35) should be almost stronger than the pure necessary condition we provided in (36).

6. Conclusions

The *non-local* feature of the integral operators defining real order derivatives is in contrast to the local behavior of the classical integer order differential operators, which can be evaluated considering values of the function under derivation in

an arbitrary small interval around the variable. This property of *memory* of the fractional derivatives leads to very complex discretizations of these operators and, as a consequence, the arithmetic cost of the corresponding algorithms increases, with respect to the methods usually employed when dealing with integer order differential equations.

In this paper we constructed a numerical scheme solving the fractional evolution-diffusion equation and we developed the corresponding classical discrete Von Neumann-type analysis that revealed pure necessary conditions of stability which, in general, are not sufficient. However this was to be expected. Indeed, from a theoretical point of view, when a Von Neumann-type analysis is carried out on finite difference schemes associated to initial-boundary values problems for parabolic equations, it leads to stability conditions that are both necessary and sufficient if the matrix associated to the scheme is symmetric. When dealing with schemes for hyperbolic equations (or, worse still, with memory in time as in our case) a symmetric matrix can almost never be expected and so only pure necessary conditions are deduced.

On the other hand, the dispersion–dissipation study for the numerical scheme highlighted that the Fourier modes do not grow in time and/or one, at least, decays when the necessary condition of stability derived from the Von Neumann-type analysis is fulfilled. Also, the scheme turned out to be dispersive, although this behavior could not be observed whenever, as it usually occurs, the dissipation hides the dispersion and the Fourier components moving at a wrong velocities are muffled.

In conclusion, the continuous and discrete evolution-diffusion equations of Dirac's type, representing a generalization of the classical evolution, diffusion and wave equations, show a dispersion–dissipation behavior in the middle between the parabolic (dissipative) and the hyperbolic one (non-dissipative). It is very typical, when dealing with fractional operators, to obtain results generalizing and interpolating the classical ones corresponding to integer order cases.

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